Meso-scale Simulations of Explosives:

A reality check

Ralph Menikoff, T-14

- Meso-scale simulations

  Continuum mechanical simulations that resolve heterogeneities

- Applied to explosives

  Burn is dominated by hot spots

    Weak ignition

    Shock desensitization

  Need to resolve hot spots

    Subgrain in extent

- Reaction rates versus burn models

  Reaction rates are for chemical processes

  Burn models are homogenized or sub-grid models

    Account for unresolved processes

- Goals

  Quantitative understanding of hot spots and burn rate

  ► Develop *improved* burn models

Burn models: state of the art ?

Currently available burn models:

- ▶ Forest Fire
- ▶ DAGMAR “improvement” based on Lagrangian analysis
- ▶ Ignition & growth
- ▶ JTF

General comments:

- Heuristic and empirical in nature

  How are model parameters determined ?

- Models work for class of problems

  Those similar to experiments used for calibration

  Same distribution of hot spots

- Threshold phenomena

  Ignition sensitivity, particularly to weak stimulus

  Needed to assess accident scenarios

  Qualitative but not quantitative

Are models adequate ?

To judge burn models

- Need suite of test problems

  Chuck Mader compiling problems this summer

  Better to have consensus among modelers and users

- Run all models on all tests

  Same model parameters for all tests

- Need to study mesh convergence

  Distinction between model vs algorithmic implementation

AMRITA environment of James Quirk would be ideal tool

- Fair comparison of models

  Change burn model leaving everything else fixed

  Grid, hydro algorithm, viscosity, EOS, etc.

- Automate running of tests

  Minimize human labor

- Standardized output

  Plots of results on fixed scale

- Open environment

  Anyone can examine source and results of tests

  Take advantage of WWW to exchange information

Additional Challenge

Predict effect of aging on explosives
or more generally,
Predict sensitivity & performance based on

- Properties of components
  HE & binder
- Micro-structure
  Grain distribution
  Defects such as voids
- Impurities
  such as RDX in HMX-based PBX

For example

Predict differences in Pop-plot for HMX-based PBXs:

PBX-9404
PBX-9501
LX-10
EDC-37

Meso-Scale Simulations

Compaction Waves in Granular Bed of HMX

Compared with gas gun experiments of Sheffield, Gustavsen et al.
"Shock Loading of Porous High Explosives"
in **High-Pressure Shock Compression of Solids IV: Response of Highly Porous Solids to Shock Compression**

LANL Shot #912 & Sandia Shot #2477
35% porosity & low impact velocity (280 m/s projectile)
Similar strength stress wave as DDT tube test of McAfee & Asay

"Compaction Wave Profiles: Simulations of Gas Gun Experiments"
http://t14web.lanl.gov/Staff/rsm/preprints.html#CmpWvPrf

Results:

- Mechanical properties
  Heterogeneities give rise to fluctuations
  Average fields have appearance of shock profiles
  Compaction wave satisfies jump conditions
- Temperature fluctuations
  Localized hot spots (tail of temperature distribution)
  Peak temperature well below melting
  Too low for burn

Homogenized model is fine for inerts but not sufficient for reactive flow

Key Issues for Reactive Simulations

- **Dissipative Mechanism**
  - ► Fluctuations are sensitive to heterogeneities & dissipation
    Reaction rate dominated by tail of temperature distribution
  - ► Dissipation predominantly near interfaces

- **Geometry**
  Granular bed is three-dimensional
  Effects distribution of contacts and voids
    Need 3-D simulations
  Heterogeneities from anisotropy

- **Computational Dilemma**
  Grain distortion vs accuracy at interface
    Eulerian algorithms can handle large distortion
    But interfaces are smeared out
  Multi-scale problem
    Resolution affects peak temperature
    Need adaptive mesh refinement

- **Material Properties**
  Significant uncertainty

- **Reaction Rate**
  Significant uncertainty

Material Properties of HMX

More important for meso-scale simulations than engineering simulations
http://t14web.lanl.gov/Staff/rsm/preprints.html#HMXmeso

- Hydrostatic EOS
  Fitting Forms for Isothermal Data (with Tommy Sewell)
  http://t14web.lanl.gov/Staff/rsm/preprints.html#IsothermFit

- Specific heat
  ▶ Critical parameter for determining hot-spot temperature
  At atmospheric pressure
  C_p increases by 50% from room temperature to δ-transition
  Variation presumably due to intra-molecular vibrations
  Also, affects Grüneisen coefficient

- Melt temperature
  At atmospheric pressure, $T_m = 550$ K
  ▶ Dependence on pressure ?
  Affects viscosity coefficient
  Model EOS accounts for latent heat <u>but not volume change</u>

- Yield strength
  From elastic precursor, 2.6 kb
  From hardness measurements, 1.3 kb
  ▶ Brittle ductile transition with confinement pressure

Reaction Rate

- Arrhenius rate, $R = (1-\lambda) Z \exp(-T/T_a)$
  R. Rogers data, Z & T_a for liquid phase
  Shock in single crystal HMX (B. Craig)
  For $P_s = 340\,\mathrm{kb} \lesssim \mathrm{P_{CJ}}$, induction time greater than 1 μs
  Orders of magnitude larger than predicted by rate constants
  ► Rate for single crystal and liquid are significantly different

- Pressure dependence of rate
  Calorimetry data indicates Z is function of P.

- Cook-off experiments
  Atmospheric pressure
  Multi-step reaction
  First step is $\beta - \delta$ transition (Henson et al.)
  Endothermic, $\Delta T = Q/C_v \approx 200\,\mathrm{K}$
  Expansion $\Delta V/V \approx 8\,\%$
  Transition time $\sim 25\,$ms at melting temperature
  and decreases with increasing temperature
  Nucleation depends on impurities/defects
  For shock heating, possibly $\beta \rightarrow$ liquid
  Co-existence curves are not known
  ► Confinement would affect transition, $\Delta P = K \Delta V/V$

Model Problem

Shock initiation, $P_s \gtrsim 100\,\text{kb}$

Dominated by void collapse (Mader)

$Re = \frac{\ell u \rho}{\mu} \gg 1$ (for $\mu = 1\,$Poise, $\ell \gtrsim 1\,\mu$m & $u = 1\,\frac{\text{mm}}{\mu\text{s}}$, $Re \gtrsim 20$)

Likely to require less resolution than weak ignition

Single Curve Build-Up Principle & Pop-Plot

1. Implosion of single pore
   - ► Reaction quenches due to expansion & heat conduction

   Hot-spot temperature & energy release as function of P_s

2. Interaction of many pore collapses

   Pressure waves from hot spots interact

   Shock heating not sufficient

3. Coupling to shock front

   As hot-spot temperature increases, induction time decreases

   and time delay for acoustic wave to reach front decreases

Shock passing over void creates hot spot
Energy release from hot spot increases shock pressure
which increase strength of hot spot
and increases even more energy
Then feedback results in build-up to detonation

Both Pop-plot data and velocity profile data from gas gun experiments